Continuum versus periodic lattice Monte Carlo approach to classical field theory

Bogdan Mihaila*
Physics Division, Argonne National Laboratory, Argonne, IL 60439

John F. Dawson†
Department of Physics, University of New Hampshire, Durham, NH 03824

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We compare the momentum space with the standard periodic lattice approach to Monte Carlo calculations in classical ϕ^4 field theory. We show that the mismatch in the initial value of $\phi^2_{\rm cl}(t)$, results in a shift in the "thermalized" value, at large times. The two approaches converge to the same result in the continuum limit.

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I. INTRODUCTION

Classical field theory in 1+1 dimensions has been used recently as a test ground for various approximation methods for calculating the dynamical evolution of a nonequilibrium system [1, 2, 3]. In classical field theory one can numerically simulate the full time evolution of the system via Monte Carlo methods [1]. Given the probability distributions in the initial state of the system, one can randomly sample the initial distributions and numerically solve the equations of motion. The time evolution of the various expectation values is then obtained by averaging over the number of independent realizations. The dynamics becomes exact in the limit when the number of initial samples goes to infinity.

It is important to be able to carry out calculations both in coordinate (lattice) and momentum space. In a lattice calculation, operators are numerically realized by using finite-difference representations of derivatives and integrals. Finite-difference methods, though leading to sparse matrices, are notoriously slow to converge. Thus the need of using higher order methods, like the nonuniform grid Chebyshev polynomial methods [4, 5] we used in the past few years, which belong to the class of spectral methods. Then the resulting matrices are less sparse, but what we apparently loose in storage requirements, we gain in speed. We do in fact keep the storage needs moderate also, as we can achieve very good accuracy with a moderate number of grid sites. Spectral methods have made possible for the first time to carry out complex dynamical calculations at next to leading order in quantum mechanics [5, 6, 7] and field theory [2].

In order to evaluate the quality of the various approximations, one needs to find ways of comparing the truncated dynamics predicted by a given approximation scheme with the exact result. Hence the importance of classical field theory where Monte Carlo methods allow us to probe the true dynamics of a hamiltonian system. In practice, the exact calculation is always carried out in two steps: First, we consider a truncated space, which is characterized by a cutoff in momentum space. Once a solution is obtained for a given finite value of the cutoff, we increase the value of the cutoff and repeat the calculation until the result becomes independent of the cutoff. This second step is what we usually refer to as *taking the continuum limit*.

Lattice and momentum space (continuum) calculations do give the same result in the continuum limit. However, in a truncated space the results will be different. Since we are trying to compare the exact dynamics of a system with the result of a non-lattice based calculation, we cannot reliably use the lattice result. Hence the need for a continuum implementation of the Monte Carlo method.

It is interesting to remark here that the study of the classical ϕ^4 field theory problem represents a warmup for the next-to-leading order studies of the quantum linear sigma model [8] and beyond. For the linear sigma model, the presence of the Landau pole will prevent us from taking the momentum cutoff to arbitrarily large values. Therefore, we are in fact less interested in the continuum limit of the problem, at least for now.

II. THE LAGRANGIAN

For a real field $\phi(x)$, the classical Lagrangian density in the $\phi^4(x)$ theory is given by:

$$\mathcal{L}(\phi,\partial_\mu\phi)=\frac{1}{2}\left[\partial_\mu\phi(x)\right]\left[\partial^\mu\phi(x)\right]-\frac{\lambda}{8}\left[\phi^2(x)-r_0^2\right]^2\,,$$

or

$$\mathcal{L}(\phi,\partial_\mu\phi) \tag{1}$$
$$=\frac{1}{2}\left\{(\partial_\mu\phi(x))(\partial^\mu\phi(x))-\mu^2\,\phi^2(x)\right\}-\frac{\lambda}{8}\,\phi^4(x)-\frac{\mu^4}{2\lambda}\,,$$

where $\mu^2=-\lambda r_0^2/2>0$. The classical equation of motion for $\phi(x)$, in 1+1 dimensions, is:

$$\left[\partial_t^2-\partial_x^2+\mu^2+\frac{\lambda}{2}\,\phi^2(x,t)\right]\phi(x,t)=0\,. \tag{2}$$

*Electronic address: bogdan.mihaila@unh.edu
†Electronic address: john.dawson@unh.edu

In order to make contact with the work of Aarts *et al* [1], in this paper we address only the symmetric case, $\langle\phi(0)\rangle = \langle\pi(0)\rangle = 0$.

III. INITIAL VALUES

Assuming that initially the system is in thermal equilibrium, the initial values $\phi(x,0)$ and $\pi(x,0) = \dot{\phi}(x,0)$ are taken from a canonical ensemble governed by a classical density distribution $\rho[\phi,\pi]$ defined as

$$\rho[\phi,\pi] = Z^{-1}(\beta_0)\, e^{-\beta_0 H[\phi,\pi]}\,, \qquad (3)$$
$$Z(\beta_0) = \prod_x \int\int \mathrm{d}\phi(x)\,\mathrm{d}\pi(x)\, e^{-\beta_0 H[\phi,\pi]}\,.$$

with $\beta_0 = 1/T_0$, and $\pi(x,t) = \dot{\phi}(x,t)$. Correspondingly, the ensemble average of a quantity $A[\phi,\pi]$ is defined by

$$\langle A[\phi,\pi]\rangle = \mathrm{Tr}\{\rho A[\phi,\pi]\} \qquad (4)$$

Following Aarts *et al* [1], we choose initial values by randomly sampling the density distribution corresponding to the free particle Hamiltonian ($\lambda = 0$). For each set of initial conditions, we time-evolve $\phi(x,t)$ using the equation of motion (2). The average value $\phi^2_{\mathrm{cl}}(t)$ is calculated as

$$\phi^2_{\mathrm{cl}}(t) = \frac{1}{M_c}\sum_{i=1}^{M_c} \lim_{L\to\infty}\frac{1}{L}\int_{-\frac{L}{2}}^{\frac{L}{2}} \phi^2(x,t)\,\mathrm{d}x\,, \qquad (5)$$

where (i) denotes the i^{th} Monte-Carlo run and M_c is the total number of Monte-Carlo runs.

IV. MOMENTUM SPACE APPROACH

In the momentum space approach one introduces the Fourier transform of the field $\tilde{\phi}(q,t)$ via

$$\phi(x,t) = \int \frac{\mathrm{d}q}{2\pi}\,\tilde{\phi}(q,t)\, e^{-\mathrm{i}qx}\,.$$

One then obtains the classical equation of motion in momentum space

$$\left[\partial_t^2 + (q^2+\mu^2)\right]\tilde{\phi}(q,t) + \frac{\lambda}{2}\int \mathrm{d}x\; e^{\mathrm{i}qx}\;\phi^3(x,t) = 0\,.$$

The equation of motion is solved by using an Euler method, where the time-differential operator is replaced by a second order difference formula, i.e.

$$\partial_t^2\tilde{\phi}(q,t) \to \left[\tilde{\phi}(q,t+\tau) - 2\,\tilde{\phi}(q,t) + \tilde{\phi}(q,t-\tau)\right]/\,\tau^2\,,$$

where τ is the time step. A momentum space cut-off is used and the system is also in a box of length L. Letting $L = Na$, and choosing our momentum to be

$$q = \frac{2\pi k}{L}, \quad k = \left\{-\frac{N}{2},\ldots,\frac{N}{2}-1\right\}\,, \qquad (6)$$

we then have that

$$\Lambda = \frac{\pi N}{L} = \frac{\pi}{a}\,, \qquad (7)$$

where Λ is the momentum cutoff and a is the lattice spacing. Then, we must take the continuum limit as

$$\int \frac{\mathrm{d}q}{2\pi}(\;) \to \lim_{\Lambda\to\infty}\int_{-\Lambda}^{\Lambda}\frac{\mathrm{d}q}{2\pi}(\;)\,.$$

In this approach, the periodic boundary assumption is implied whenever we perform numerical Fourier transforms and convolutions, the continuum Fourier being replaced by the discrete one.

We will choose the initial values for $\tilde{\phi}(q,0)$ and $\tilde{\pi}(q,0)$ to be solutions of the unperturbed Hamiltonian

$$H_0 = \frac{1}{2}\int \mathrm{d}x\left\{\pi_0^2(x) + \left[\partial_x\phi_0(x)\right]^2 + \mu^2\,\phi_0^2(x)\right\}\,, \qquad (8)$$

where $\pi_0(x,t) = \dot{\phi}_0(x,t)$. The corresponding equation of motion in momentum space is

$$\left[\partial_t^2 + \omega_q^2\right]\,\tilde{\phi}_0(q,t) = 0\,, \qquad (9)$$

with the dispersion relation

$$\omega_q^2 \;=\; q^2 + \mu^2\,. \qquad (10)$$

General solutions of Eq. (9) are of the form:

$$\tilde{\phi}_0(q,t) \;=\; \frac{1}{\sqrt{2\omega_q}}\left[\tilde{a}_q\, e^{-\mathrm{i}\omega_q t} \;+\; \tilde{a}^*_{-q}\, e^{\mathrm{i}\omega_q t}\right]\,,$$

and

$$\tilde{\pi}_0(q,t) = \dot{\tilde{\phi}}_0(q,t) \;=\; \frac{1}{i}\sqrt{\frac{\omega_q}{2}}\,\left[\tilde{a}_q\, e^{-\mathrm{i}\omega_q t} \;-\; \tilde{a}^*_{-q}\, e^{\mathrm{i}\omega_q t}\right]\,.$$

We can now calculate the classical density matrix as

$$\rho_0[a_m,a_m^*] = \frac{1}{Z_0(\beta_0)}\prod_k e^{-\beta_0\omega_{q_k}\,(x^2_{q_k}+y^2_{q_k})/L}\,, \qquad (11)$$
$$Z_0(\beta_0) = \prod_x\int\int \mathrm{d}\phi_0(x)\,\mathrm{d}\pi_0(x)\, e^{-\beta_0 H_0[\phi_0,\pi_0]}\,.$$

where we have put $a_{q_k} = x_{q_k} + \mathrm{i}y_{q_k}$. Hence, the symmetric case scenario, $\langle\phi(0)\rangle = \langle\pi(0)\rangle = 0$, implies that x_{q_k} and y_{q_k} are uniform random deviates between 0.0 and 1.0 .

Using Eq. (4) with the density distribution given by (11), we obtain

$$\langle\tilde{a}_{q_k}\tilde{a}_{q_{k'}}\rangle \;=\; \langle\tilde{a}^*_{q_k}\tilde{a}^*_{q_{k'}}\rangle \;=\; 0\,,$$
$$\langle\tilde{a}^*_{q_k}\tilde{a}_{q_{k'}}\rangle \;=\; \langle\tilde{a}_{q_k}\tilde{a}_{q_{k'}}\rangle \;=\; n_{q_k}(\beta_0)\;\delta_{k,k'}/L\,,$$

where $n_q(\beta_0) = 1/(\beta_0 \omega_q)$. Note that $n_q(\beta_0)$ is the high temperature limit of the classical Bose-Einstein occupation number distribution. Finally, we obtain

$$\langle \phi^2(0) \rangle \;=\; \frac{1}{\beta_0}\,\frac{1}{L}\sum_k \frac{1}{\omega_{q_k}^2} \;=\; \frac{1}{\mu\beta_0}\, I(\mu,\Lambda)\;,$$
$$\langle \pi^2(0) \rangle \;=\; \frac{1}{\beta_0}\,\frac{1}{L}\sum_k \;=\; \frac{1}{\beta_0}\,\frac{1}{a}\;,$$

with

$$I(\mu,\Lambda) \;=\; \frac{1}{\pi}\,\arctan(\Lambda/\mu)\;. \qquad (12)$$

Thus, for a given cut-off in momentum space, we have

$$\langle \phi^2(0) \rangle \;=\; \frac{1}{\mu\beta_0\,\pi}\,\arctan(\Lambda/\mu)\;. \qquad (13)$$

In the limit when $\Lambda \to \infty$, we obtain $\langle \phi^2(0) \rangle = 1/(2\mu\beta_0)$.

V. PERIODIC LATTICE APPROACH

For the lattice formalism, we follow closely the approach presented in Reference [1]. We discretize the continuum equations by using a lattice in coordinate space with spacing a and periodic boundary conditions. The differential operators are replaced by second order difference formulas:

$$\partial_x^2\phi(x,t) \to \Big[\phi(x+a,t) - 2\,\phi(x,t) + \phi(x-a,t)\Big] \,/\, a^2\;,$$
$$\partial_t^2\phi(x,t) \to \Big[\phi(x,t+\tau) - 2\,\phi(x,t) + \phi(x,t-\tau)\Big] \,/\, \tau^2\;.$$

The dispersion relation is modified due to the Laplacian on the lattice and becomes

$$\omega_{\hat{q}}^2 = \hat{q}^2 + \mu^2, \quad \hat{q}^2 = \frac{2}{a^2}(1-\cos aq)\;, \qquad (14)$$

with $a = \pi/\Lambda$. The momentum q takes the same finite number of discrete values, see Eq. (6). The relationship between the cutoffs in the two approaches is given by

$$\lim_{L\to\infty} \int_{-\frac{L}{2}}^{\frac{L}{2}} (\;) \to \lim_{N\to\infty} \frac{1}{Na} \sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} (\;) \to \lim_{\Lambda\to\infty} \int_{-\Lambda}^{\Lambda} \frac{\mathrm{d}q}{2\pi} (\;)\;.$$

The initial conditions are generated by sampling the initial probability distribution of the unperturbed system just as in the continuum case, with the formal difference that we replace the values of the momenta q_k by the shifted values $\hat{q}_k$. Then, the initial expectation value becomes

$$\langle \phi^2(0) \rangle \;=\; \frac{1}{\beta_0}\,\frac{1}{L}\sum_k \frac{1}{\omega_{\hat{q}_k}^2} \;=\; \frac{1}{\mu\beta_0}\, \hat{I}(\mu,a)\;,$$

where

$$\hat{I}(\mu,a) \;=\; \frac{1}{2\sqrt{1+(\mu a/2)^2}}\;. \qquad (15)$$

Thus, for a given lattice spacing $a = \pi/\Lambda$, we obtain

$$\langle \phi^2(0) \rangle \;=\; \frac{1}{\mu\beta_0}\,\frac{1}{2\sqrt{1+(\mu a/2)^2}}\;. \qquad (16)$$

In the limit when $a \to 0$ $(\Lambda \to \infty)$, we recover the continuum limit $\langle \phi^2(0) \rangle = 1/(2\mu\beta_0)$. However, for a given momentum space cutoff Λ, the values of $\langle \phi^2(0) \rangle$ given by Eqs. (13) and (16) are not the same (see Fig. 1). This is an artifact of solving the equations of motions on the lattice and requiring $\phi(x,t)$ to satisfy periodic boundary conditions. As a consequence, one cannot directly compare continuum and lattice calculations.

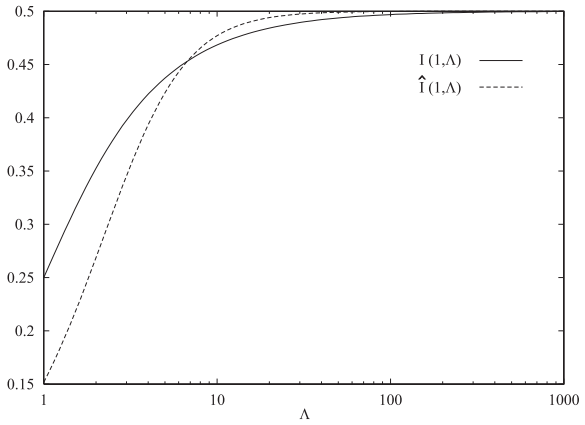

FIG. 1: $I(\mu = 1, \Lambda)$ and $\hat{I}(\mu = 1, \Lambda)$ as a function of Λ.

VI. RESULTS

We choose to illustrate the approaches presented above, for a set of parameters which allows us to compare with results available in the literature [1]. We have $\lambda = 1/3$, $\mu = 1$, $\Lambda = 4\pi$, $T_0 = 5.03891094$. Then, the initial condition corresponding to the momentum space approach is $\langle \phi^2(0) \rangle = 2.39208677$, as obtained from Eq. (13), while the numerically calculated initial average is $\phi^2_{\rm cl}(0) = 2.39187089$, for a 0.009% error. In turn the lattice calculation produces the continuum limit $\langle \phi^2(0) \rangle = 2.5$, provided that one choose the lattice spacing $a = 0.25$. The lattice spacing is subsequently left unchanged, even though one may vary the number of lattice sites, and implicitly the lattice size (see Eq. (7)).

The numerical methods used for the numerical implementation of the two methods are well under control. In Fig. 2 we show the Monte-Carlo value of $\phi^2_{\rm cl}(t)$, as defined in Eq. (5), obtained using the periodic lattice approach. The error lines represent coordinate average deviations of the runs as a function of t. Similar results are obtained using the momentum space approach.

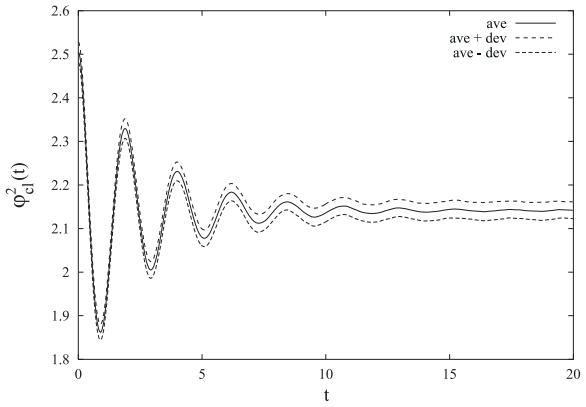

FIG. 2: Monte-Carlo calculation of $\phi^2_{\rm cl}(t)$ versus t.

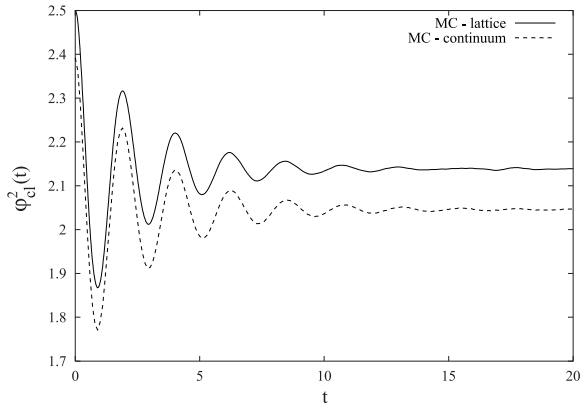

FIG. 3: Comparison of the *lattice* and the *continuum* Monte Carlo results, respectively.

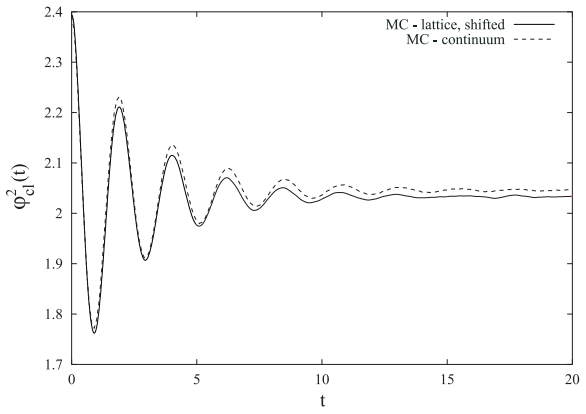

FIG. 4: Comparison of the *shifted lattice* and the *continuum* Monte Carlo results, respectively.

In Fig. 3 we compare the calculated time dependence of $\phi^2_{\rm cl}(t)$, obtained using the periodic and momentum space, respectively. In fact, the main source of difference resides in the different initial values. To illustrate this aspect we depict the same numerical results in Fig. 4, but shift the lattice curve such that we match the initial value of $\phi^2_{\rm cl}(t)$.

VII. CONCLUSIONS

In this paper we have discussed two approaches of obtaining the dynamical evolution of a classical system, one based on a lattice formulation in coordinate space, the other in momentum space. Both methods require the assumption of periodic boundary conditions, but the different levels at which this assumption is made, allows the momentum space approach to avoid certain artifacts of the lattice based method. In particular the intrinsic mismatch in initial conditions at finite cut-off values, results in different values of the "thermalized" field, at large times. The discrepancy is worse for smaller values of the cut-off, but the two approaches converge to the same result in the continuum limit. The mismatch in initial conditions is due to the fact that by using a finite difference approximation for the spatial derivative operator together with the assumption of periodic boundary conditions on the lattice, we have in fact introduced a approximation of the dispersion relation (see Eq. (14) – lattice, and Eq. (10) – continuum), which is now viewed as an expansion in the lattice spacing a. In order to improve the quality of the spatial derivative approximation in the lattice case, one would normally have to take the limit when the lattice spacing a goes to zero. We are however prevented from doing that, since the choice of the momentum cut-off Λ also determines the choice of the lattice spacing $a = \pi/\Lambda$. Consequently we cannot improve the agreement of the lattice dispersion relation with the continuum for a given momentum space cut-off. The momentum space (continuum) approach does not exhibit this limitation.

One may think of modifying the unperturbed Hamiltonian in order to effectively obtain a higher-order approximation of the dispersion relation while still having the same type of equations of motion, similar to the improved action framework in lattice QCD. This would result in new values $\hat{q}^2$, and would require cancelling the various orders of a in a rigorous fashion. (The standard lattice calculation introduces values of $\hat{q}^2$ which differ from q^2 already at order a^2.) However, this is beyond the scope of the present work, and since we are in fact able to obtain an exact solution for the continuum problem, we merely state here the differences between the lattice and the continuum approach.

Acknowledgments

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